

Faddeev calculation for breakup neutron-deuteron scattering at 14.1 MeV lab energy

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Abstract. A new computational method for solving the nucleon-deuteron breakup scattering problem has been applied to study the inelastic neutron-deuteron scattering on the basis of the configuration-space Faddeev equations. This method is based on the spline-decomposition in the angular variable and on a generalization of the Numerov method for the hyperradius. The Merkuriev-Gignoux-Laverne approach has been generalized for arbitrary nucleon-nucleon potentials and with an arbitrary number of partial waves. Neutron-deuteron observables at the incident nucleon energy 14.1 MeV have been calculated using the charge-independent AV14 nucleon-nucleon potential. Results have been compared with those of other authors and with experimental neutron-deuteron scattering data.

1. Introduction

The last two decades brought tremendous progress in both theoretical and experimental study of nucleon-deuteron scattering. More accurate experimental data were compared with rigorous calculations in the framework of the Faddeev equations with high-precision nucleon-nucleon potentials also including model three-nucleon forces [1, 2]. Nucleon-nucleon (NN) potentials used in rigorous three-nucleon (3N) calculations are charge-independent AV14 [3], AV18 [4], CD-Bonn [5] and several Nijmegen potentials [6]. Among three-nucleon forces (3NF) are Tucson-Melbourne (TM) and its various modifications [7], and Urbana potentials [8]. Based on the chiral effective field theory (EFT) NN and 3N potentials have been constructed [9] and used in rigorous 3N calculations [2].

In spite of these enormous achievements in the 3N studies, there are several important cases where the rigorous 3N calculations have failed to explain the data [10] and these discrepancies are established with very high precision. Among the most important discrepancies are the A_y puzzle in nucleon-deuteron (Nd) elastic scattering [11], the star configuration in the Nd breakup reaction [12] and the quasi-free scattering (QFS) cross section [1].

Recent calculations of the proton-deuteron breakup cross-section, and tensor analyzing power data for a symmetric constant relative energy (SCRE) geometry reported in [13] revealed a serious disagreement between the theory and experimental data. Inclusion of the TM or Urbana 3NF did not solve the problem. The chiral EFT showed the same deviations from the data. Including the Coulomb force partially improved the situation for the cross section. On the other hand predictions in [14] with the 3NF forces and Coulomb interaction taken into account showed a good agreement with the data. At the same time, the recent study of Nd breakup in symmetric star configurations based on Faddeev calculations with CD-Bonn NN potential [15] showed significant discrepancy for nn QFS configuration and a good agreement with cross-section data in the case of pn QFS breakup geometry. Thus the situation with theoretical predictions for the 3N observables remains still far from completely resolved. This motivates us to continue searching for new computational procedures and input potentials, which may allow to overcome the mentioned disagreements.

In this article we present an alternative method for the study of the neutron-deuteron (nd) system based on the direct numerical solution of the Faddeev equations in configuration space. This approach was initiated by Merkuriev et al. (MGL) [16] who derived general formulae for nd breakup scattering. This method has been initially applied to the study of nd and pd elastic and breakup scattering with nuclear interaction limited only to S-waves and with simple NN potentials [17]. In the present work we generalize the MGL approach to any high precision realistic potentials for nd inelastic processes.

This paper is organized as follows: in section 2 we describe calculations in configuration space starting with the general formalism in subsection 2.1 followed by

Numerov method in subsection 2.2. Our novel method for solution is given in subsection 2.3. Formulae for calculating elastic and breakup amplitudes in MGL basis are presented in section 2.4. Comparison of our results with the previous calculations and with the data are discussed in section 3. Finally, discussion and conclusion are given in sections 4 and 5.

2. Three-nucleon Faddeev calculation in configuration space - our new computational method

2.1. Formalism

The starting point for studying interactions between nucleons in three-body systems is the solution of the Schrödinger equation $H\Psi = E\Psi$ for nuclear Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^3 \nabla_i^2 + \sum_{j<k} V_{jk} \left(+ \sum_{j<k<l} V_{jkl} \right), \quad (1)$$

where V_{jk} and V_{jkl} are the two- and three-nuclear potentials, respectively. In this study we neglected three-nucleon forces V_{jkl} .

Writing the total wave function as

$$\Psi = \Phi_1 + \Phi_2 + \Phi_3 = (1 + P^+ + P^-)\Phi_1, \quad (2)$$

the Schrödinger equation for three identical particles can be reduced into a single Faddeev equation, which in Jacobi's vectors \vec{x}_1, \vec{y}_1 has the form

$$\left[-\frac{\hbar^2}{m} (\Delta_{\vec{x}_1} + \Delta_{\vec{y}_1}) + V(\vec{x}_1) - E \right] \Phi(\vec{x}_1, \vec{y}_1) = -V(\vec{x}_1)(P^+ + P^-)\Phi(\vec{x}_1, \vec{y}_1), \quad (3)$$

where the operators P^\pm are the cyclic permutation operators for the three particles which interchange any pair of nucleons ($P^+ : 123 \rightarrow 231, P^- : 123 \rightarrow 312$), and $\hbar^2/m = 41.47 \text{ MeV} \cdot \text{fm}^2$. As independent coordinates, we take the Jacobi vectors $\vec{x}_\alpha, \vec{y}_\alpha$. For the pair $\alpha=1$, they are related to particle coordinates by the formulas:

$$\vec{x}_1 = \vec{r}_2 - \vec{r}_3, \quad \vec{y}_1 = \frac{\vec{r}_2 + \vec{r}_3}{2} - \vec{r}_1, \quad (4)$$

for $\alpha=2,3$ one has to make cyclic permutations of the indexes in Eq.(5). The Jacobi vectors with different α 's are linearly related by the orthogonal transformation

$$\begin{pmatrix} \vec{x}_\alpha \\ \vec{y}_\alpha \end{pmatrix} = \begin{pmatrix} C_{\alpha\beta} & S_{\alpha\beta} \\ -S_{\alpha\beta} & C_{\alpha\beta} \end{pmatrix} \begin{pmatrix} \vec{x}_\beta \\ \vec{y}_\beta \end{pmatrix}, \quad C_{\alpha\beta}^2 + S_{\alpha\beta}^2 = 1, \quad (5)$$

where

$$C_{\alpha\beta} = -\sqrt{\frac{m_\alpha m_\beta}{(M-m_\alpha)(M-m_\beta)}}, \quad S_{\alpha\beta} = (-)^{\beta-\alpha} \text{sgn}(\beta - \alpha) \sqrt{1 - C_{\alpha\beta}^2}, \quad (6)$$

$$M = \sum_{\alpha=1}^3 m_\alpha.$$

To perform numerical calculations for arbitrary nuclear potential, we use MGL approach [16]. To make the angular analysis of Eq.(3), we use a basis proposed in [16]. This basis is intermediate between LS and Jj coupling schemes.

Let: $\vec{\sigma}$, \mathbf{l} and $\mathbf{J} = \vec{\sigma} + \mathbf{l}$ be the spin, orbital and total angular momenta of the pair

23. $\mathbf{s} = \mathbf{1}/2 + \mathbf{J}$ the total "spin" of the system 123 considering the pair 23 as a particle with "spin" \mathbf{J} . $\vec{\lambda}$ the orbital momentum conjugate to \mathbf{y} , that is of the relative motion of particle 1 respective to the c.m of pair 23. $\mathbf{M} = \vec{\lambda} + \mathbf{s}$ the total angular momentum with its z -projection M_z . To this we have to add the isospin part. If the isospin of the pair 23 is \mathbf{t} , then the total isospin is $\mathbf{T} = \mathbf{1}/2 + \mathbf{t}$ with its projection T_z . Since in the nd case $T = 1/2$ it need not be shown explicitly. The set of quantum numbers $\{\lambda s l \sigma J\} \equiv \alpha$ defines a state in this basis.

Correspondingly in this basis the spin-angular-isospin eigenfunctions have the form

$$Z_\alpha(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = \langle \hat{\mathbf{x}}, \hat{\mathbf{y}} | \alpha \rangle = [Y^\lambda(\hat{\mathbf{y}}) \otimes [\chi^{1/2} \otimes \mathcal{Y}_{l\sigma}^J(\hat{\mathbf{x}})]^s]^{M, M_z} \eta_{1/2, t}^{T, T_z} \quad (7)$$

For nd scattering the Faddeev equations for partial components can be written in the following form (here we omit the index 1):

$$\begin{aligned} & \left[E + \frac{\hbar^2}{m}(\partial_x^2 + \partial_y^2) - v_\alpha^\lambda(x, y) \right] \Phi_\alpha^{\lambda_0, s_0, M_0}(x, y) = \\ & \sum_\beta v_{\alpha\beta}(x) \left[\Phi_\beta^{\lambda_0, s_0, M_0}(x, y) + \int_{-1}^1 du \sum_\gamma g_{\beta\gamma}(y/x, u) \Phi_\gamma^{\lambda_0, s_0, M_0}(x', y') \right]. \end{aligned} \quad (8)$$

The geometrical function $g_{\beta\gamma}(x, y, u)$ is the representative of the permutation operator $P^+ + P^-$ in MGL basis [16]:

$$\begin{aligned} & g_{\alpha'\alpha}(y/x, u) = g_{\alpha'\alpha}(\theta, u) = g_{\alpha'\alpha}(\theta, \theta') \\ & = (-1)^{\lambda+\lambda'+J+J'} [(2J+1)(2J'+1)(2s+1)(2s'+1)]^{1/2} \sum_{LS} (2S+1)(2L+1) \\ & \left\{ \begin{matrix} l & \sigma & J \\ 1/2 & s & S \end{matrix} \right\} \left\{ \begin{matrix} l' & \sigma' & J' \\ 1/2 & s' & S \end{matrix} \right\} \left\{ \begin{matrix} \lambda & l & L \\ S & M & s \end{matrix} \right\} \left\{ \begin{matrix} \lambda' & l' & L \\ S & M & s' \end{matrix} \right\} \\ & < \chi_{1/2\sigma'}^S \eta_{1/2,t'}^T | P^+ | \chi_{1/2\sigma}^S \eta_{1/2,t}^T > h_{\lambda'l'\lambda l}^L(y/x, u). \end{aligned} \quad (9)$$

Function h is the representative of the permutation operator $P^+ + P^-$ in the $\lambda + l = L$ basis:

$$\begin{aligned} & h_{\lambda'l'\lambda l}^L(y/x, u) = h_{\lambda'l'\lambda l}^L(\theta, u) = h_{\lambda'l'\lambda l}^L(\theta, \theta') \\ & = \frac{xy}{x'y'} (-1)^{l+L} \frac{(2\lambda+1)(2l+1)}{2^{\lambda+l}} [(2\lambda)!(2l)!(2\lambda'+1)(2l'+1)]^{1/2} \\ & \sum_{k=0} (-1)^k (2k+1) P_k(u) \sum_{\lambda_1+\lambda_2=\lambda, l_1+l_2=l} \frac{y^{\lambda_1+l_1} x^{\lambda_2+l_2}}{y'^{\lambda} x'^l} (-1)^{l_2} \\ & \frac{(\sqrt{3})^{\lambda_2+l_1}}{[(2\lambda_1)!(2\lambda_2)!(2l_1)!(2l_2)!]^{1/2}} \sum_{\lambda''l''} (2\lambda''+1)(2l''+1) \\ & \left(\begin{matrix} \lambda_1 & l_1 & \lambda'' \\ 0 & 0 & 0 \end{matrix} \right) \left(\begin{matrix} \lambda_2 & l_2 & l'' \\ 0 & 0 & 0 \end{matrix} \right) \left(\begin{matrix} k & \lambda'' & \lambda' \\ 0 & 0 & 0 \end{matrix} \right) \left(\begin{matrix} k & l'' & l' \\ 0 & 0 & 0 \end{matrix} \right) \\ & \left\{ \begin{matrix} l' & \lambda' & L \\ \lambda'' & l'' & k \end{matrix} \right\} \left\{ \begin{matrix} \lambda_1 & \lambda_2 & \lambda \\ l_1 & l_2 & l \\ \lambda'' & l'' & L \end{matrix} \right\}. \end{aligned} \quad (10)$$

The index k runs from zero to $(\lambda' + l' + \lambda + l)/2$. The (...) are the $3j$ symbols:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_3+m_3+2j_1} \frac{1}{\sqrt{2j_3+1}} C_{j_1-m_1, j_2-m_2}^{j_3 m_3}.$$

The centrifugal potential is

$$v_\alpha^\lambda = \frac{\hbar^2}{m} \left[\frac{l(l+1)}{x^2} + \frac{\lambda(\lambda+1)}{y^2} \right], \quad (11)$$

and nucleon-nucleon potentials are $v_{\alpha\alpha'}(x) = \langle \alpha | v(\mathbf{x}) | \alpha' \rangle = \delta_{\lambda\lambda'} \delta_{ss'} \delta_{\sigma\sigma'} \delta_{JJ'} v_{ll'}^{\sigma J}$, where $v_{ll'}^{\sigma J}$ are the potential representatives in the two-body basis $\mathcal{Y}_{l\sigma}^{JJz}(\hat{\mathbf{x}})$ (most often abbreviated as $^{2\sigma+1}l_J$).

The set of partial differential equation Eqs.(8) must be solved for functions satisfying the regularity conditions

$$\Phi_\alpha^{\lambda_0 s_0 M_0}(0, \theta) = \Phi_\alpha^{\lambda_0 s_0 M_0}(\rho, 0) = \Phi_\alpha^{\lambda_0 s_0 M_0}(\rho, \pi/2) = 0 \quad (12)$$

The asymptotic conditions for nd breakup scattering has the following form [18]:

$$\begin{aligned} \Phi_\alpha^{\lambda_0 s_0 M_0}(x, y) \sim & \left\{ \left[\delta_{\lambda\lambda_0} \delta_{ss_0} \delta_{\sigma 1} \delta_{j1} \hat{j}_\lambda(qy) + \left(-\hat{y}_\lambda(qy) + i\hat{j}_\lambda(qy) \right) a_{\lambda s \lambda_0 s_0}^{M_0} \right] \psi_l(x) \right. \\ & \left. + O(y^{-1}) \right\} + A_{\alpha, \lambda_0 s_0}^{M_0}(\theta) \frac{e^{iKX}}{\sqrt{X}} + O(X^{-3/2}), \end{aligned} \quad (13)$$

$$X^2 = x^2 + y^2, \quad K^2 = \frac{mE}{\hbar^2}, \quad x \text{ finite}, \quad y \rightarrow \infty,$$

where ψ_l is l -th component of deuteron wave function ($l=0,2$), and \hat{j} and \hat{y} are the regularized spherical Bessel functions.

The matrix of partial elastic amplitudes a has the structure

$$a_{\lambda s \lambda_0 s_0}^{M_0} = \frac{\eta \exp(2i\delta) - 1}{2i}, \quad (14)$$

where η and δ are the inelasticities and scattering phases. In Eq.(13) the amplitudes $A_{\alpha, \lambda_0 s_0}^{M_0}$ are related with physical breakup amplitudes. The inelastic scattering amplitudes are given by the sum

$$\mathcal{A}_{\alpha, \lambda_0 s_0}^{M_0}(\theta) = A_{\alpha, \lambda_0 s_0}^{M_0}(\theta) + \int_{-1}^1 du \sum_\beta g_{\alpha\beta}(\theta, u) A_{\beta, \lambda_0 s_0}^{M_0}(\theta'). \quad (15)$$

To simplify the numerical solution of Eqs.(8), we write down Eqs.(8) in the polar coordinate system ($\rho^2 = x^2 + y^2$ and $\tan \theta = y/x$):

$$\begin{aligned} & \left[E + \frac{\hbar^2}{m} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{4\rho^2} \right) - v_\alpha^\lambda(\rho, \theta) \right] U_\alpha^{\lambda_0 s_0 M_0}(\rho, \theta) = \\ & \sum_\beta v_{\alpha\beta}(\rho, \theta) \left[U_\beta^{\lambda_0 s_0 M_0}(\rho, \theta) + \int_{-1}^1 du \sum_\gamma g_{\beta\gamma}(\theta, u, \theta'(\theta, u)) U_\gamma^{\lambda_0 s_0 M_0}(\rho, \theta') \right]. \end{aligned} \quad (16)$$

Here the first derivative in the radius is eliminated by the substitution $U = \rho^{-1/2} \Phi$. In Eqs.(15-16) the angular variable θ' is defined by

$$\cos^2 \theta'(u, \theta) = \frac{1}{4} \cos^2 \theta - \frac{\sqrt{3}}{2} \cos \theta \sin \theta \cdot u + \frac{3}{4} \sin^2 \theta. \quad (17)$$

2.2. Numerov method

Modification of the Numerov method for the set of the differential equations (16) does not present any difficulties in principle. As is well known, the Numerov method is an efficient algorithm for solving second-order differential equations. The important feature of the equations for the application of Numerov's method is that the first derivative has to be absent. The aim of this method is to improve the accuracy of the finite-difference approximation for the second derivative. Starting from the Taylor expansion truncated after the sixth derivative for two points adjacent to x_n , that is for x_{n-1} and x_{n+1} one sums these two expansions to give a new computational formula that includes the fourth derivative. This derivative can be found by straightforward differentiation of the second derivative from the initial second-order differential equation (see the details in [19]). For brevity, we omit the corresponding derivation and present only the final formula of Numerov's method for Eqs. (16), not indicating indices $\lambda_0 s_0 M_0$:

$$\begin{aligned}
& -\left[E + \frac{12}{(\Delta\rho)^2} + \left(1 + \frac{2\Delta\rho}{\rho_j}\right)\frac{T_\alpha(\theta)}{\rho_j^2}\right]U_\alpha(\rho_{j-1}, \theta) = \\
& \sum_\beta (v_{\alpha\beta}(\rho_j, \theta) - \Delta\rho v'_{\alpha\beta}(\rho_j, \theta))(U_\beta(\rho_{j-1}, \theta) + \sum_\gamma \int_{\theta^-}^{\theta^+} d\theta' g_{\beta\gamma}(\theta, \theta')U_\gamma(\rho_{j-1}, \theta')) \\
& -2\left[5E - \frac{12}{(\Delta\rho)^2} + \left(5 + \frac{3\Delta\rho}{\rho_j}\right)\frac{T_\alpha(\theta)}{\rho_j^2}\right]U_\alpha(\rho_j, \theta) \\
& + \sum_\beta (10v_{\alpha\beta}(\rho_j, \theta) + (\Delta\rho)^2 v''_{\alpha\beta}(\rho_j, \theta))(U_\beta(\rho_j, \theta) + \sum_\gamma \int_{\theta^-}^{\theta^+} d\theta' g_{\beta\gamma}(\theta, \theta')U_\gamma(\rho_j, \theta')) \\
& -\left[E + \frac{12}{(\Delta\rho)^2} + \left(1 - \frac{2\Delta\rho}{\rho_j}\right)\frac{T_\alpha(\theta)}{\rho_j^2}\right]U_\alpha(\rho_{j+1}, \theta) \\
& + \sum_\beta (v_{\alpha\beta}(\rho_j, \theta) + \Delta\rho v'_{\alpha\beta}(\rho_j, \theta))(U_\beta(\rho_{j+1}, \theta) + \sum_\gamma \int_{\theta^-}^{\theta^+} d\theta' g_{\beta\gamma}(\theta, \theta')U_\gamma(\rho_{j+1}, \theta')) = 0,
\end{aligned} \tag{18}$$

where

$$T_\alpha(\theta) = \frac{\partial^2}{\partial\theta^2} - \frac{l(l+1)}{\cos^2\theta} - \frac{\lambda(\lambda+1)}{\sin^2\theta} + \frac{1}{4}.$$

In Eq. (18) ρ_j is the j -th current point for hyperradius $\rho \in (0, R_{max})$ in the radial grid ($j = 1, 2, \dots, N_\rho$), $\Delta\rho_j$ is the radial step-interval.

To ensure the accuracy of order $(\Delta\theta)^4$ for the approximation in the angular variable, Hermitian splines of the fifth degree have been used (see Ref. [20]). These splines are local and each spline $S_{\sigma i}(x)$ is defined for x belonging to two adjacent subintervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$. Their analytical form is fixed by the following smoothness conditions:

$$S_{\sigma i}(x_{i-1}) = 0, \quad S_{\sigma i}(x_{i+1}) = 0, \quad \sigma = 0, 1, 2, \tag{19}$$

and

$$\begin{aligned}
S_{0i}(x_i) &= 1, & S'_{0i}(x_i) &= 0, & S''_{0i}(x_i) &= 0, \\
S_{1i}(x_i) &= 0, & S'_{1i}(x_i) &= 1, & S''_{1i}(x_i) &= 0, \\
S_{2i}(x_i) &= 0, & S'_{2i}(x_i) &= 0, & S''_{2i}(x_i) &= 1.
\end{aligned} \tag{20}$$

Expansion of the Faddeev component into basis of the Hermitian splines has the following form:

$$U_\alpha(\rho, \theta) = \sum_{\sigma=0}^2 \sum_{j=0}^{N_\theta+1} S_{\sigma j}(\theta) C_{\alpha j}^\sigma(\rho), \quad (21)$$

where $N_\theta + 1$ is the number of internal subintervals for the angular variable $\theta \in [0, \pi/2]$.

To reduce the resulting equation (18) to an algebraic problem, one should explicitly calculate the derivatives of NN potentials $v_{\alpha\beta}(\rho, \theta)$ with respect to ρ and the second derivatives of splines $S_{\sigma j}(\theta)$ with respect to θ . It is convenient to express the second derivative of component U_α with respect to θ through U_α itself using Eq.(21). Upon substituting the spline expansion (21) and expression for its second derivative into Eqs.(18), we use a collocation procedure with three Gaussian quadrature points per subinterval. As the number of internal breakpoints for angular variable θ is equal to N_θ , the basis of quintic splines consists of $3N_\theta + 6$ functions. Three of them should be excluded using the last two regularity conditions from (12) and continuity of the first derivative in θ of the Faddeev component at either $\theta = 0$ or $\theta = \pi/2$, as the collocation procedure yields $3N_\theta + 3$ equations. Finally Eqs.(18) for the Faddeev components are to be written as the following matrix equation:

$$\begin{aligned} A_1 U_1 + G_1 U_2 &= 0, \\ B_j U_{j-1} + A_j U_j + G_j U_{j+1} &= 0, \quad j = 2, \dots, N_\rho - 1, \\ B_{N_\rho} U_{N_\rho-1} + A_{N_\rho} U_{N_\rho} &= -G_{N_\rho} U_{N_\rho+1}. \end{aligned} \quad (22)$$

In this equation vector $U_k = U(\rho_k)$ has dimension N_{in} and matrices A, B, G , derived from Eq.(18), have dimension $N_{in} \times N_{in}$ where $N_{in} = N_\alpha \times N_c$, and N_α is the number of partial waves and $N_c = 3N_\theta + 3$ is the number of collocation points in the angular variable θ .

2.3. The novel method of solution

To derive equations for calculation of breakup and amplitudes, the method of partial inversion [19] has been applied. We write down Eq.(22) in a matrix form:

$$(D * U)_i = -\delta_{iN_\rho} G_{N_\rho} U_{N_\rho+1}. \quad (23)$$

Here matrix D is of dimension $N_\rho N_{in} \times N_\rho N_{in}$, and N_ρ is the number of breakpoints in the hyperradius ρ . The form of this equation results from keeping the incoming wave in the asymptotic conditions (13). As a consequence, the right hand part of Eq. (22) has a single nonzero term marked with index $N_\rho + 1$. Sparse (tri-block-diagonal) structure of matrix D optimizes considerably the inversion problem. Hyperradius $\rho_{n+1} = R_{max}$, where R_{max} is the cutoff radius at which the asymptotic conditions Eqs. (13) are implemented. By formal inversion of the matrix D in Eq. (23), the solution of the problem may be written in the following form:

$$U_j = -D_{jn}^{-1} G_{N_\rho} U_{N_\rho+1}, \quad j = 1, 2, \dots, N_\rho. \quad (24)$$

In Eq. (24) one should consider the last two components of vector U :

$$\begin{aligned} U_{N_\rho-1} &= -D_{N_\rho-1 N_\rho}^{-1} G_{N_\rho} U_{N_\rho+1} \\ U_{N_\rho} &= -D_{N_\rho N_\rho}^{-1} G_{N_\rho} U_{N_\rho+1}. \end{aligned} \quad (25)$$

Provided R_{max} is large enough, the vectors $U_{N_\rho-1}, U_{N_\rho}$ on the left side of Eqs.(25) may be replaced by the corresponding vectors obtained by evaluating Eqs. (13) at the radii $\rho = \rho_{N_\rho-1}$ and $\rho = \rho_{N_\rho}$. As a result we obtain a set of linear equations for the unknown amplitudes a and \mathcal{A} :

$$\begin{aligned} a \cdot v_{N_\rho-1} + m_{N_\rho-1} \cdot \mathcal{A} &= \mathcal{F}_{N_\rho-1} \\ a \cdot v_{N_\rho} + m_{N_\rho} \cdot \mathcal{A} &= \mathcal{F}_{N_\rho}. \end{aligned} \quad (26)$$

For the sake of brevity, we do not display here the explicit form of vectors v_j, \mathcal{F}_j and matrices m_j . As $R_{max} \rightarrow \infty$ the set of equations (26) has a constant a as a solution. At finite R_{max} its solution is a vector a with generally different components corresponding to different angles. We follow the method of S.P. Merkuriev [18], which consists in selecting the components of a in the region of the maximum of the deuteron wave function, where a turns out to be independent of the angle.

Furthermore, we propose a new method for a more adequate calculation of the amplitudes. The set of linear equations (26) is over determined, since the number of equations is $2 \cdot N_{in}$ and the number of unknowns is $N_{in}+1$. Therefore it is natural to use the least-squares method (LSM). One can apply it by two ways. In the first one, it is needed to express the breakup amplitude \mathcal{A} from the lower equation (26) and substitute it into the upper one. As a result one has the following expression:

$$a \cdot \mathbf{v} = \mathbf{F}, \quad (27)$$

where vectors are defined as follows: $\mathbf{v} = v_{n-1} - m_{n-1} m_n^{-1} v_n$, $\mathbf{F} = \mathcal{F}_{n-1} - m_{n-1} m_n^{-1} \mathcal{F}_n$. According to LSM one should to minimize the following functional

$$\|a \cdot \mathbf{v} - \mathbf{F}\|^2 = \min. \quad (28)$$

Differentiating this expression in $\text{Re } a$ and $\text{Im } a$ we obtain

$$a = \frac{(\mathbf{v}^*, \mathbf{F})}{(\mathbf{v}^*, \mathbf{v})}, \quad (29)$$

where (ξ^*, f) is an ordinary scalar product.

In the second way, it is needed to express the elastic amplitude a from the lower equation (26) using the scalar product:

$$a = \frac{(v_n^*, \mathcal{F}_n - m_n \mathcal{A})}{(v_n^*, v_n)}. \quad (30)$$

Substituting a from Eq. (30) into the equation (26), leads to the set of linear equations

$$m_{n-1} \mathcal{A} - v_{n-1} \frac{(v_n^*, m_n \mathcal{A})}{(v_n^*, v_n)} = \mathcal{F}_{n-1} - v_{n-1} \frac{(v_n^*, \mathcal{F}_n)}{(v_n^*, v_n)}. \quad (31)$$

The explicit form of Eq. (31) is as follows

$$\sum_{j=1}^{N_c} \left\{ m_{n-1,ij} - \frac{v_{n-1,i}}{(v_n^*, v_n)} \sum_{k=1}^{N_c} v_{n,k}^* m_{n,kj} \right\} \mathcal{A}_j = \mathcal{F}_{n-1,i} - v_{n-1,i} \frac{(v_n^*, \mathcal{F}_n)}{(v_n^*, v_n)}, \quad i = 1, \dots, N_c. \quad (32)$$

Solving the set in Eq. (32), we get the breakup amplitude \mathcal{A} . Substituting the obtained breakup amplitude into Eq. (30), one may compute the elastic amplitude a . Note that one can apply Eq. (30) to calculate the elastic amplitude a either in the components or via a scalar product. In the first case, the components of a are practically equal to a constant for all angles $\theta \in (0, \pi/2)$ and this constant coincides with the value of a calculated by using the scalar product to the fourth decimal. It should also be noted that the elastic amplitudes calculated by the method from [18] and LSM coincide with this constant to the same accuracy. To control the accuracy of calculations, all methods are used.

2.4. Observables

To calculate observables for elastic scattering of nucleon from deuteron in the direction $\hat{\mathbf{q}}'$ (initial direction $\hat{\mathbf{q}}$ is along the z-axis), one has to derive the equation for the elastic amplitude as a function of scattering angle. Omitting this derivation, we represent the final expression for this amplitude in MGL basis:

$$\hat{a}_{\sigma'_z, J'_z, \sigma_z, J_z}(\hat{\mathbf{q}}') = \sum_{\lambda'} \sum_{\lambda_s} \sum_{\lambda_s'} i^{\lambda-\lambda'} \sqrt{\frac{2\lambda+1}{4\pi}} C_{\lambda' M_z - \sigma'_z - J'_z, s' \sigma'_z + J'_z}^{MM_z} C_{\lambda 0, s \sigma_z + J_z}^{MM_z} C_{1/2 \sigma'_z, 1 J'_z}^{s' \sigma'_z + J'_z} C_{1/2 \sigma, 1 J_z}^{s \sigma_z + J_z} Y_{\lambda' M_z - \sigma'_z - J'_z}(\hat{\mathbf{q}}') a_{\lambda' s' \lambda s}^M, \quad (33)$$

with $M_z = \sigma_z + J_z$.

In Eq. (33) $\sigma' \sigma'_z(\sigma, \sigma_z)$ and $J' J'_z(J J_z)$ are spin and its projection for incoming (scattered) nucleon, and the deuteron in the rest (scattered deuteron), respectively. Thus, the nuclear part of the elastic amplitude is a $(2 \times 2) \otimes (3 \times 3)$ matrix in the spin states of nucleon and deuteron, depending on the spherical angles θ and ϕ .

The spin elastic observable formulas can be taken from the review [1]. They are expressed via spin 2×2 matrices σ_i for the nucleon and 3×3 matrices \mathcal{P}_i and \mathcal{P}_{ik} for the deuteron. The latter are related to the deuteron spin matrices S_i :

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (34)$$

One has $\mathcal{P}_i = S_i$, $\mathcal{P}_{ik} = 3/2(S_i S_k + S_k S_i)$, $\mathcal{P}_{zz} = 3S_z S_z - 2I$, and $\mathcal{P}_{xx} - \mathcal{P}_{yy} = 3(S_x S_x - S_y S_y)$.

Nucleon analyzing powers A_k are

$$A_k = \frac{\text{Tr}(\hat{a} \sigma_k \hat{a}^\dagger)}{\text{Tr}(\hat{a} \hat{a}^\dagger)}. \quad (35)$$

If the scattering plane is the xy plane and the y axis points to the direction $\mathbf{q} \times \mathbf{q}'$ then due to parity conservation $A_x = A_z = 0$ and the only non-zero component is A_y . The deuteron vector and tensor analyzing powers are defined as

$$A_k = \frac{\text{Tr}(\hat{a}\mathcal{P}_k\hat{a}^\dagger)}{\text{Tr}(\hat{a}\hat{a}^\dagger)}, \quad A_{jk} = \frac{\text{Tr}(\hat{a}\mathcal{P}_{jk}\hat{a}^\dagger)}{\text{Tr}(\hat{a}\hat{a}^\dagger)}. \quad (36)$$

Parity conservation puts A_x, A_z, A_{xy} and A_{yz} to zero. So the non-vanishing and independent analyzing powers are defined by

$$iT_{11} = \frac{\sqrt{3}}{2}A_y, \quad T_{20} = \frac{1}{\sqrt{2}}A_{zz}, \quad T_{21} = -\frac{1}{\sqrt{3}}A_{xz}, \quad T_{22} = \frac{1}{2\sqrt{3}}(A_{xx} - A_{yy}). \quad (37)$$

Also spin transfer coefficients are given in the review [1]. They have the same structure as the quantities above, with slightly different matrices to be inserted between \hat{a} and \hat{a}^\dagger .

In the case of Nd breakup scattering expression for physical breakup amplitude to calculate breakup observables has much more complex form. Below we present the main details of its derivation. The asymptotic of the wave function with the given incident plane wave is defined as follows

$$\Psi_{q,s_0,s_{0z}}(\mathbf{x}, \mathbf{y}) = \frac{e^{iKX}}{X^{5/2}} \frac{4\pi}{q} \sum_{\lambda_0, \lambda_{0z}, M_0, M_{0z}} c_{\lambda_0, s_0, M_0}^{\lambda_0, s_0, M_0}(\hat{\mathbf{q}}) \sum_{\alpha} \frac{\mathcal{A}_{\alpha}^{\lambda_0 s_0, M_0}(\theta)}{\sin \theta \cos \theta} Z_{\alpha}(\hat{\mathbf{y}}, \hat{\mathbf{x}}), \quad (38)$$

where the initial plane wave has the form

$$c_{\lambda_0 s_0 M_0}^{\lambda_0 s_0 M_0}(\hat{\mathbf{q}}) = i^{\lambda_0} C_{\lambda_0 \lambda_{0z} s_0 s_{0z}}^{M_0 M_{0z}} [Y_{\lambda_0 \lambda_{0z}}]^*(\hat{\mathbf{q}}), \quad (39)$$

and $Z_{\alpha}(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ are the spin-angular-isospin eigenfunctions.

The exponential factor is multiplied by the function depending only on angles, that are directions of vectors \mathbf{q} , \mathbf{x} and \mathbf{y} . This gives a probability to find the breakup particles at given directions and so with the amplitude for the breakup with given directions of \mathbf{p}' and \mathbf{q}' . So the breakup amplitude is

$$\mathcal{A}_{q,s_0,s_{0z}}(\mathbf{p}', \mathbf{q}') = \frac{4\pi}{q} \sum_{\lambda_0, \lambda_{0z}, M_0, M_{0z}} c_{\lambda_0, s_0, M_0}^{\lambda_0, s_0, M_0}(\hat{\mathbf{q}}) \sum_{\alpha} \frac{\mathcal{A}_{\alpha}^{\lambda_0 s_0, M_0}(\theta)}{\sin \theta \cos \theta} Z_{\alpha}(\hat{\mathbf{q}}', \hat{\mathbf{p}}'), \quad (40)$$

where now $\theta = \arctan(q'/p')$

The only thing necessary to pass to the formula for the breakup is to project this amplitude onto the state with given projections of spins of the three particles μ_1, μ_2, μ_3 . This will obviously be given by introducing into the sum over α in Eq. (40) the projection

$$d_{\alpha, \mu_1 \mu_2 \mu_3}^{M_0 M_{0z}}(\hat{\mathbf{p}}', \hat{\mathbf{q}}') = \langle \mu_1 \mu_2 \mu_3 | Z_{\alpha}(\hat{\mathbf{q}}', \hat{\mathbf{p}}') \rangle. \quad (41)$$

As the result we get the breakup scattering amplitude as a function of final nucleon momenta in the following form

$$\begin{aligned} & \mathcal{A}(\hat{\mathbf{p}}', \hat{\mathbf{q}}', \mu_1 \tau_1 \mu_2 \tau_2 \mu_3 \tau_3 | \mathbf{q}, s_0, s_{0z}) \\ &= \frac{4\pi}{q} \sum_{\alpha, \pi, \lambda_0, M_0, \lambda_{0z}, M_{0z}} d_{\mu_1 \tau_1 \mu_2 \tau_2 \mu_3 \tau_3, \alpha}^{M_0, M_{0z}}(\hat{\mathbf{p}}', \hat{\mathbf{q}}') \frac{\mathcal{A}_{\alpha, \lambda_0, s_0}^{M_0}(\theta')}{\sin \theta' \cos \theta'} c_{\lambda_0 s_0 M_0}^{\lambda_0 s_0 M_0}(\hat{\mathbf{q}}') \end{aligned} \quad (42)$$

where μ_i and τ_i $i = 1, 2, 3$ are the spin and isospin projections of the three nucleons, $\theta' = \arctan(q'/p')$, and summation goes over $\lambda_{0z} + s_{0z} = M_{0z}$. $\mathcal{A}_{\alpha, \lambda_{0z}, s_{0z}}^{M_0}$ is the spherical inelastic amplitude defined in Eq. (15). The d -coefficients are

$$d_{\mu_1 \tau_1 \mu_2 \tau_2 \mu_3 \tau_3, \alpha}^{M_0, M_{0z}}(\hat{\mathbf{p}}', \hat{\mathbf{q}}') = (-1)^{\lambda+J+M-1/2} [(2J+1)(2S+1)]^{1/2} C_{\frac{1}{2}\mu_2, \frac{1}{2}\mu_3}^{\sigma\mu_2+\mu_3} \\ C_{\frac{1}{2}\tau_2, \frac{1}{2}\tau_3}^{t\tau_2+\tau_3} C_{\frac{1}{2}-\frac{1}{2}-\tau_2-\tau_3, t\tau_2+\tau_3}^{\frac{1}{2}-\frac{1}{2}} \sum_{LS} [(2L+1)(2S+1)]^{1/2} C_{\frac{1}{2}\mu_1, \sigma\mu_2+\mu_3}^{SS_z} C_{LM_{0z}-S_z, SS_z}^{M_0 M_{0z}} \\ \left\{ \begin{matrix} l & \sigma & J \\ 1/2 & s & S \end{matrix} \right\} \left\{ \begin{matrix} \lambda & l & L \\ S & M & s \end{matrix} \right\} \mathcal{Y}_{\lambda l}^{L, M_{0z}-S_z}(\hat{\mathbf{q}}', \hat{\mathbf{p}}') \quad (43)$$

where $S_z = \mu_1 + \mu_2 + \mu_3$ and $t=0$ or 1 according to antisymmetry condition $l + \sigma + t$ odd.

The breakup differential cross-section is then

$$\frac{d^5\sigma}{d^3p'd^2\hat{\mathbf{q}}'} = \frac{4q'}{3K^3q} |\mathcal{A}(\hat{\mathbf{p}}', \hat{\mathbf{q}}', \mu_1\tau_1\mu_2\tau_2\mu_3\tau_3|\mathbf{q}, s_0, s_{0z})|^2 \quad (44)$$

Note that $d^3p'q'd^2\hat{\mathbf{q}}' = p'd^2\hat{p}'d^3q'$

This formula may be transformed to the form which is used by the experimentalists in the lab. system.

$$\frac{d^5\sigma}{dSd^2\hat{\mathbf{k}}_1d^2\hat{\mathbf{k}}_2} = \frac{\sqrt{3}mk_1^2k_2^2}{qK^3\sqrt{D}} |\mathcal{A}(\hat{\mathbf{p}}', \hat{\mathbf{q}}', \mu_1\tau_1\mu_2\tau_2\mu_3\tau_3|\mathbf{q}, s_0, s_{0z})|^2 \quad (45)$$

where

$$D = k_1^2(2k_2 - \hat{\mathbf{k}}_2(\mathbf{k}_{lab} - \mathbf{k}_1))^2 + k_2^2(2k_1 - \hat{\mathbf{k}}_1(\mathbf{k}_{lab} - \mathbf{k}_2))^2 \quad (46)$$

and S is the arc lenght along the allowed curve in the $E_1 - E_2$ plane:

$$dS = dE_1 \sqrt{1 + \left(\frac{k_2}{k_1} \frac{2k_1 - \hat{\mathbf{k}}_1(\mathbf{k}_{lab} - \mathbf{k}_2)}{2k_2 - \hat{\mathbf{k}}_2(\mathbf{k}_{lab} - \mathbf{k}_1)} \right)^2} \quad (47)$$

This cross-section refers to the breakup experiment in which all individual spins and isospins of the final nucleons and the spin of the initial neutron-deuteron system are given. The unpolarized cross-section with the isospin projections of the final nucleons given is obtained by summing Eq. (45) over μ_1, μ_2, μ_3 and averaging over s_0 and its projections s_{0z} :

$$\frac{d^5\sigma}{dSd^2\hat{\mathbf{k}}_1d^2\hat{\mathbf{k}}_2} = \frac{\sqrt{3}mk_1^2k_2^2}{qK^3\sqrt{D}} \frac{1}{6} \sum_{\mu_1, \mu_2, \mu_3, s_0, s_{0z}} |\mathcal{A}(\hat{\mathbf{p}}', \hat{\mathbf{q}}', \mu_1\tau_1\mu_2\tau_2\mu_3\tau_3|\mathbf{q}, s_0, s_{0z})|^2 \quad (48)$$

To write this expression in a more convenient form, one can introduce a matrix between initial and final spins:

$$\hat{\mathcal{A}}(\hat{\mathbf{p}}', \hat{\mathbf{q}}'|\mathbf{q})_{\mu_1, \mu_2, \mu_3 | s_0, s_{0z}} \equiv \mathcal{A}(\hat{\mathbf{p}}', \hat{\mathbf{q}}', \mu_1\tau_1\mu_2\tau_2\mu_3\tau_3|\mathbf{q}, s_0, s_{0z}) \quad (49)$$

In terms of this matrix the unpolarised cross-section can be written as

$$\frac{d^5\sigma}{dS d^2\hat{\mathbf{k}}_1 d^2\hat{\mathbf{k}}_2} = \frac{\sqrt{3} m k_1^2 k_2^2}{q K^3 \sqrt{D}} \frac{1}{6} \text{Tr}\{\hat{\mathcal{A}}^\dagger \hat{\mathcal{A}}\} \quad (50)$$

Using this matrix one can write all polarization observables in the same form as for the elastic channel. In particular the final proton analyzing power will be given by the formula

$$A_k = \frac{\text{Tr}\{\hat{\mathcal{A}}^\dagger \sigma_k^{(1)} \hat{\mathcal{A}}\}}{\text{Tr}\{\hat{\mathcal{A}}^\dagger \hat{\mathcal{A}}\}}, \quad (51)$$

where $\sigma_{\mu'_1 \mu_1}$ is the spin matrix of the 1st nucleon, supposed to be proton ($\tau_1 = +1/2$).

3. Results

We present our results for the differential cross section, nucleon analyzing power A_y , and deuteron vector iT_{11} for nd elastic scattering at 14.1 MeV in Figs. 1–3. In all our calculations we used the AV14 NN potential. The total angular momentum of the pair of nucleons j_{23} has been taken up to 3 and all values of the total three-nucleon angular momentum M up to 13/2 with both parity values (± 1) have been taken into account (up to 62 partial waves in all).

Fig. 1 shows our results for elastic differential cross sections along with the prediction of the Bochum group Ref. [21] using the charge-dependent AV18 NN potential. In Fig. 2 our results for nucleon analyzing power are shown together with the prediction of the Bochum group and experimental data from [22]. In general the agreement between our calculations of A_y and those of the Bochum group is satisfactory, since using different NN potentials may explain small differences between these calculations around the maximum values of A_y (Fig. 2).

Our predictions for the deuteron analyzing power iT_{11} and those of the Grenoble group [23] are presented in Fig. 3 along with the experimental data [24]. Again there is a small disagreement between two calculations which can be explained by the use of two different type of NN potentials. The results of the Grenoble group have been obtained with NN interactions of de Tourreil and Sprung, effective in the states $^1S_0, ^3S_1, ^3D_1, ^1P_1$, and $^3P_{0,1,2}$.

For nd breakup scattering at 14.1 MeV, our preliminary results for the breakup differential cross section and nucleon analyzing power A_y under FSI configuration are shown in Figs. 4,5 along with the experimental data [25]. Results for A_y are presented together with the calculations of Witala et al. [26] using the Paris NN potential and Bonn potential of version A and B with total two-nucleon angular momentum $j \leq 2$. Thus in their work up to 34 partial wave states have been taken into account for each total angular momentum J and parity states.

4. Discussion

Our results for nd elastic scattering at 14.1 MeV and those from the Bochum and Grenoble group are in fair agreement. Some differences can be attributed to smaller values of the total two-nucleon angular momentum j taken into account in their calculation as well as to different NN potentials used. In the energy region of tens MeV [22] and [24] theoretical predictions are 25-30% lower than the experimental data.

For nd breakup observables our predictions compare only qualitatively with the experimental data and predictions for A_γ of the Bochum group. Still the positions of the peaks in the breakup angular distribution are correct. For the nucleon analyzing power the deep minimum at arc length S equal to 7 in our results disagrees with predictions for A_γ from [26].

5. Conclusion

For nd elastic observables at 14.1 MeV acceptable agreement (in view of different NN potentials) between predictions of our calculations and those of the Bochum and Grenoble group demonstrates the soundness of our novel method providing thereby a new approach for calculating three-nucleon scattering. Our approach can and will be used to include the Coulomb force. It is well-known that Nd polarization observables are the magnifying glass for studying 3P_J NN states and calculations which rigorously include nuclear and electromagnetic interactions are very important.

Our next step is to study pd breakup scattering using a new and more accurate version of the Faddeev equations in configuration space. In presence of the Coulomb interaction serious changes are to be made in view of p and n being different particles, so that use of the isotopic formalism becomes unreasonable. As a result the Faddeev equations in configuration space derived by S.P. Merkuriev *et al.* in [17] become only approximate. Probably the error of their calculations of the elastic pd scattering amplitudes is not significant. However in the case of pd breakup scattering one has to use both charge-dependent NN AV18 potential and the new correct Faddeev equations.

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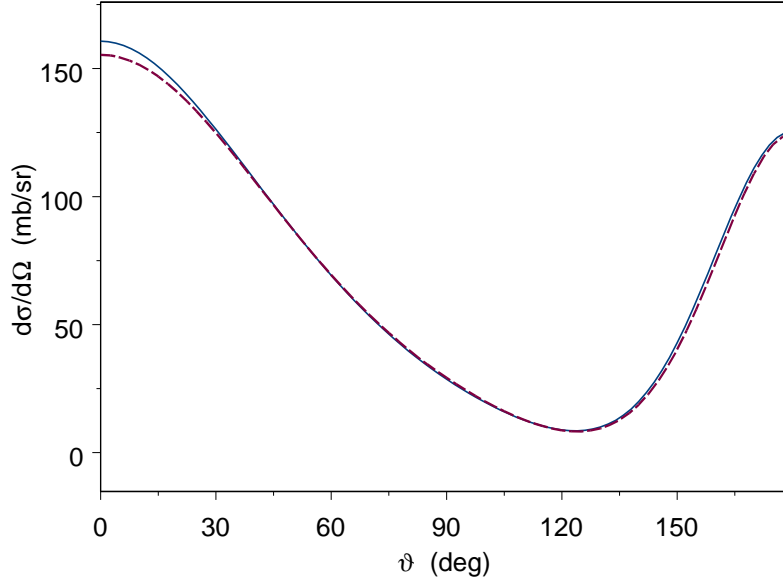


Figure 1. The differential cross section for nd scattering at $E_{\text{lab}}=14.1$ MeV. The solid line is our results. The dashed line corresponds to prediction of the Bochum group Ref. [21].

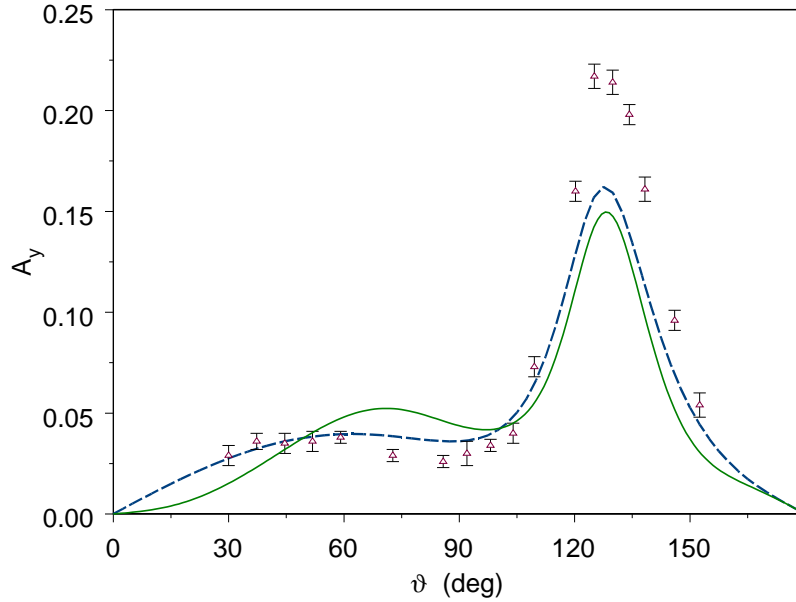


Figure 2. The nucleon analyzing power A_y for nd scattering at $E_{\text{lab}} = 14.1$ MeV. The solid line is our results. The dashed one is results of the Bochum group Ref. [21]. The experimental data are from Ref. [22].

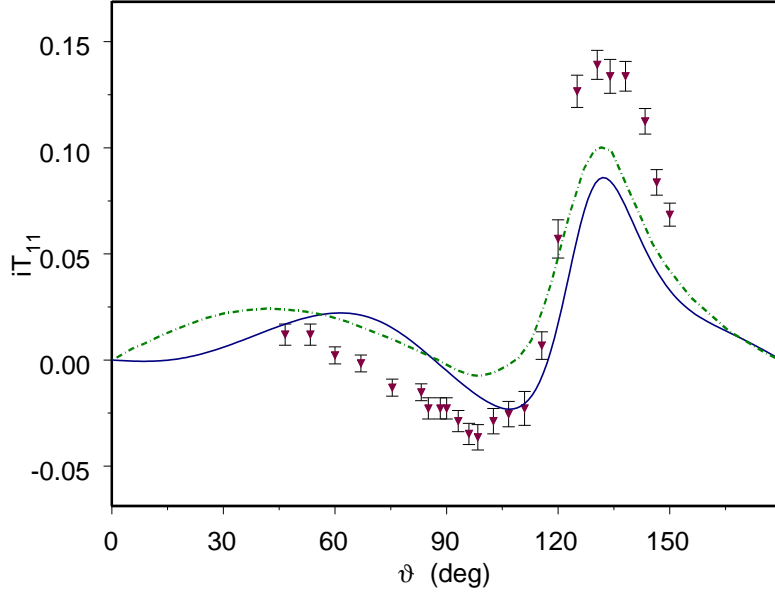


Figure 3. The deuteron analyzing power iT_{11} for nd scattering at $E_{\text{lab}} = 14.1$ MeV. The dot-dashed line is prediction of the Grenoble Group with SSC NN interaction Ref. [23]. The proton-deuteron data at $E_{\text{lab}} = 15.0$ MeV are from Ref. [24].

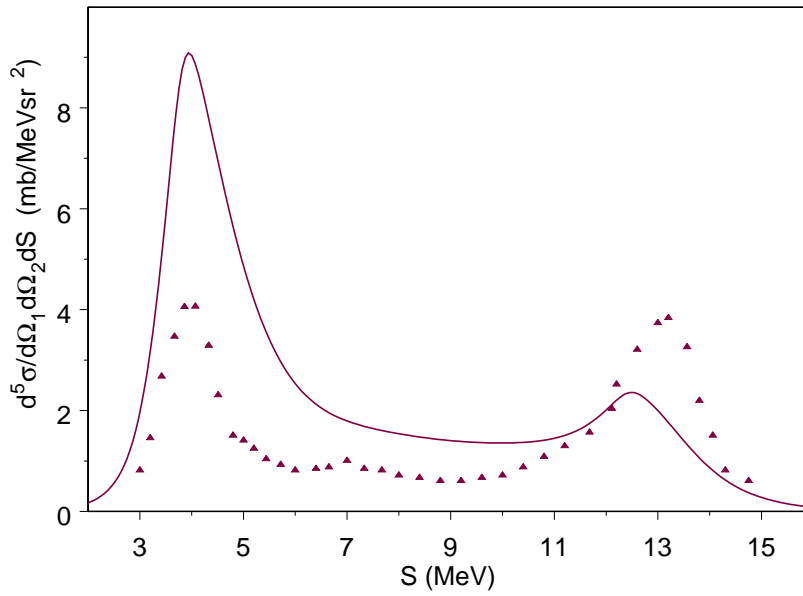


Figure 4. nd breakup differential cross section as a function of the arc length S under FSI configuration ($\theta_1 = 52.6^\circ$, $\theta_2 = 40.5^\circ$, $\phi_{12} = 180^\circ$) at $E_{\text{lab}} = 14.1$ MeV. The proton-deuteron experimental data denoted by solid triangles are from Ref. [25].

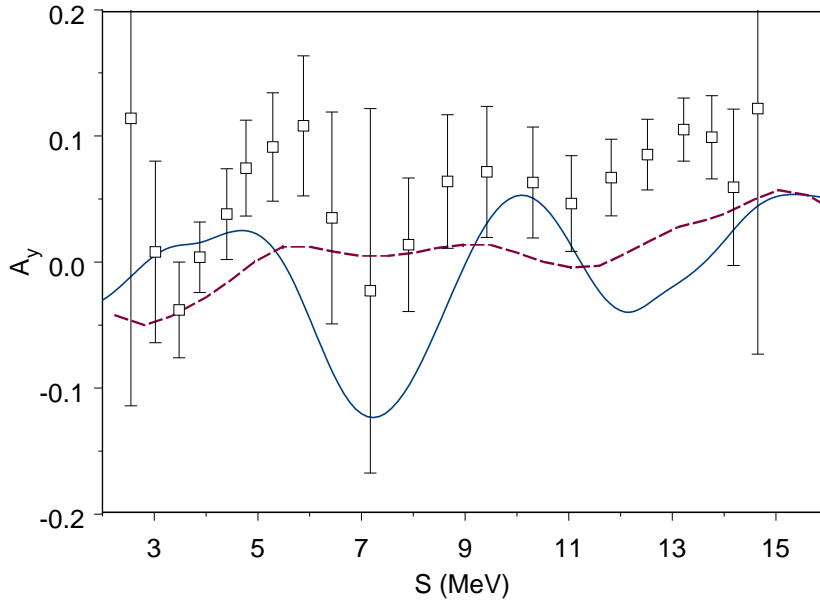


Figure 5. The nucleon analyzing power as a function of the arc length S under FSI configuration ($\theta_1 = 52.6^\circ$, $\theta_2 = 40.5^\circ$, $\phi_{12} = 180^\circ$) at $E_{\text{lab}} = 14.1$ MeV. The solid line is our results. The dashed one is results of Ref. [26]. The proton-deuteron experimental data denoted by open squares are from Ref. [25].